MSG No. 74.562 I_bmma [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `mmm'`

No.	position	mapping
1	$\left[0,\ \frac{3}{4},\ 0\right]$	`[1,4,6,7,18,19,21,24]`
2	$\left[0,\ \frac{1}{4},\ 0\right]$	`[2,3,5,8,17,20,22,23]`
3	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}\right]$	`[9,12,14,15,26,27,29,32]`
4	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[10,11,13,16,25,28,30,31]`

Table 2: Wyckoff site: `4b`, site symmetry: `mmm'`

No.	position	mapping
1	$\left[0,\ \frac{3}{4},\ \frac{1}{2}\right]$	`[1,4,6,7,18,19,21,24]`
2	$\left[0,\ \frac{1}{4},\ \frac{1}{2}\right]$	`[2,3,5,8,17,20,22,23]`
3	$\left[\frac{1}{2},\ \frac{1}{4},\ 0\right]$	`[9,12,14,15,26,27,29,32]`
4	$\left[\frac{1}{2},\ \frac{3}{4},\ 0\right]$	`[10,11,13,16,25,28,30,31]`

Table 3: Wyckoff site: `4c`, site symmetry: `mm'm'`

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[1,2,5,6,19,20,23,24]`
2	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[3,4,7,8,17,18,21,22]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[9,10,13,14,27,28,31,32]`
4	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[11,12,15,16,25,26,29,30]`

Table 4: Wyckoff site: `4d`, site symmetry: `mm'm'`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,2,5,6,19,20,23,24]`
2	$\left[0,\ \frac{1}{2},\ 0\right]$	`[3,4,7,8,17,18,21,22]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,10,13,14,27,28,31,32]`
4	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[11,12,15,16,25,26,29,30]`

Table 5: Wyckoff site: `8e`, site symmetry: `.2/m.`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[1,7,11,13]`
2	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[2,8,12,14]`

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[3,5,9,15]`
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[4,6,10,16]`
5	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[17,23,27,29]`
6	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[18,24,28,30]`
7	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[19,21,25,31]`
8	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[20,22,26,32]`

Table 6: Wyckoff site: `8f`, site symmetry: `.2/m'.`

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	`[1,11,23,29]`
2	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	`[2,12,24,30]`
3	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[3,9,21,31]`
4	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[4,10,22,32]`
5	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	`[5,15,19,25]`
6	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	`[6,16,20,26]`
7	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[7,13,17,27]`
8	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[8,14,18,28]`

Table 7: Wyckoff site: `8g`, site symmetry: `mm2`

No.	position	mapping
1	$\left[0, \frac{3}{4}, z\right]$	`[1,4,6,7]`
2	$\left[0, \frac{1}{4}, -z\right]$	`[2,3,5,8]`
3	$\left[\frac{1}{2}, \frac{1}{4}, z+\frac{1}{2}\right]$	`[9,12,14,15]`
4	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}-z\right]$	`[10,11,13,16]`
5	$\left[0, \frac{1}{4}, z\right]$	`[17,20,22,23]`
6	$\left[0, \frac{3}{4}, -z\right]$	`[18,19,21,24]`
7	$\left[\frac{1}{2}, \frac{3}{4}, z+\frac{1}{2}\right]$	`[25,28,30,31]`
8	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}-z\right]$	`[26,27,29,32]`

Table 8: Wyckoff site: `8h`, site symmetry: `mm'2'`

No.	position	mapping
1	$[0, 0, z]$	`[1,6,20,23]`
2	$[0, 0, -z]$	`[2,5,19,24]`
3	$\left[0, \frac{1}{2}, -z\right]$	`[3,8,18,21]`
4	$\left[0, \frac{1}{2}, z\right]$	`[4,7,17,22]`
5	$\left[\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}\right]$	`[9,14,28,31]`

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[10,13,27,32]`
7	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[11,16,26,29]`
8	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[12,15,25,30]`

Table 9: Wyckoff site: `8i`, site symmetry: `2'mm'`

No.	position	mapping
1	$\left[x,\ \frac{3}{4},\ 0\right]$	`[1,7,18,24]`
2	$\left[x,\ \frac{1}{4},\ 0\right]$	`[2,8,17,23]`
3	$\left[-x,\ \frac{1}{4},\ 0\right]$	`[3,5,20,22]`
4	$\left[-x,\ \frac{3}{4},\ 0\right]$	`[4,6,19,21]`
5	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}\right]$	`[9,15,26,32]`
6	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[10,16,25,31]`
7	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{2}\right]$	`[11,13,28,30]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{2}\right]$	`[12,14,27,29]`

Table 10: Wyckoff site: `8j`, site symmetry: `2m'm'`

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,2,23,24]`
2	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[3,4,21,22]`
3	$[-x,\ 0,\ 0]$	`[5,6,19,20]`
4	$\left[x,\ \frac{1}{2},\ 0\right]$	`[7,8,17,18]`
5	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,10,31,32]`
6	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	`[11,12,29,30]`
7	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[13,14,27,28]`
8	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[15,16,25,26]`

Table 11: Wyckoff site: `8k`, site symmetry: `m2'm'`

No.	position	mapping
1	$[0,\ y,\ 0]$	`[1,6,19,24]`
2	$[0,\ -y,\ 0]$	`[2,5,20,23]`
3	$\left[0,\ y+\frac{1}{2},\ 0\right]$	`[3,8,17,22]`
4	$\left[0,\ \frac{1}{2}-y,\ 0\right]$	`[4,7,18,21]`
5	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[9,14,27,32]`
6	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[10,13,28,31]`
7	$\left[\frac{1}{2},\ y,\ \frac{1}{2}\right]$	`[11,16,25,30]`
8	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}\right]$	`[12,15,26,29]`

Table 12: Wyckoff site: `8l`, site symmetry: `m2'm'`

No.	position	mapping
1	$\left[\frac{1}{2},\, y,\, 0\right]$	`[1,6,19,24]`
2	$\left[\frac{1}{2},\, -y,\, 0\right]$	`[2,5,20,23]`
3	$\left[\frac{1}{2},\, y+\frac{1}{2},\, 0\right]$	`[3,8,17,22]`
4	$\left[\frac{1}{2},\, \frac{1}{2}-y,\, 0\right]$	`[4,7,18,21]`
5	$\left[0,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	`[9,14,27,32]`
6	$\left[0,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	`[10,13,28,31]`
7	$\left[0,\, y,\, \frac{1}{2}\right]$	`[11,16,25,30]`
8	$\left[0,\, -y,\, \frac{1}{2}\right]$	`[12,15,26,29]`

Table 13: Wyckoff site: `16m`, site symmetry: `.2.`

No.	position	mapping
1	$\left[\frac{1}{4},\, y,\, \frac{1}{4}\right]$	`[1,11]`
2	$\left[\frac{1}{4},\, -y,\, \frac{3}{4}\right]$	`[2,12]`
3	$\left[\frac{3}{4},\, y+\frac{1}{2},\, \frac{3}{4}\right]$	`[3,9]`
4	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, \frac{1}{4}\right]$	`[4,10]`
5	$\left[\frac{3}{4},\, -y,\, \frac{3}{4}\right]$	`[5,15]`
6	$\left[\frac{3}{4},\, y,\, \frac{1}{4}\right]$	`[6,16]`
7	$\left[\frac{1}{4},\, \frac{1}{2}-y,\, \frac{1}{4}\right]$	`[7,13]`
8	$\left[\frac{1}{4},\, y+\frac{1}{2},\, \frac{3}{4}\right]$	`[8,14]`
9	$\left[\frac{1}{4},\, y+\frac{1}{2},\, \frac{1}{4}\right]$	`[17,27]`
10	$\left[\frac{1}{4},\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	`[18,28]`
11	$\left[\frac{3}{4},\, y,\, \frac{3}{4}\right]$	`[19,25]`
12	$\left[\frac{3}{4},\, -y,\, \frac{1}{4}\right]$	`[20,26]`
13	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	`[21,31]`
14	$\left[\frac{3}{4},\, y+\frac{1}{2},\, \frac{1}{4}\right]$	`[22,32]`
15	$\left[\frac{1}{4},\, -y,\, \frac{1}{4}\right]$	`[23,29]`
16	$\left[\frac{1}{4},\, y,\, \frac{3}{4}\right]$	`[24,30]`

Table 14: Wyckoff site: `16n`, site symmetry: `..m'`

No.	position	mapping
1	$[x,\, y,\, 0]$	`[1,24]`
2	$[x,\, -y,\, 0]$	`[2,23]`
3	$\left[-x,\, y+\frac{1}{2},\, 0\right]$	`[3,22]`
4	$\left[-x,\, \frac{1}{2}-y,\, 0\right]$	`[4,21]`
5	$[-x,\, -y,\, 0]$	`[5,20]`
6	$[-x,\, y,\, 0]$	`[6,19]`
7	$\left[x,\, \frac{1}{2}-y,\, 0\right]$	`[7,18]`
8	$\left[x,\, y+\frac{1}{2},\, 0\right]$	`[8,17]`
9	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}\right]$	`[9,32]`

continued ...

Table 14

No.	position	mapping
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[10,31]
11	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}\right]$	[11,30]
12	$\left[\frac{1}{2}-x,\ -y,\ \frac{1}{2}\right]$	[12,29]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[13,28]
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[14,27]
15	$\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}\right]$	[15,26]
16	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}\right]$	[16,25]

Table 15: Wyckoff site: 16o, site symmetry: m..

No.	position	mapping
1	$[0,\ y,\ z]$	[1,6]
2	$[0,\ -y,\ -z]$	[2,5]
3	$\left[0,\ y+\frac{1}{2},\ -z\right]$	[3,8]
4	$\left[0,\ \frac{1}{2}-y,\ z\right]$	[4,7]
5	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[9,14]
6	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[10,13]
7	$\left[\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[11,16]
8	$\left[\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[12,15]
9	$\left[0,\ y+\frac{1}{2},\ z\right]$	[17,22]
10	$\left[0,\ \frac{1}{2}-y,\ -z\right]$	[18,21]
11	$[0,\ y,\ -z]$	[19,24]
12	$[0,\ -y,\ z]$	[20,23]
13	$\left[\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[25,30]
14	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[26,29]
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[27,32]
16	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[28,31]

Table 16: Wyckoff site: 16p, site symmetry: .m.

No.	position	mapping
1	$\left[x,\ \frac{3}{4},\ z\right]$	[1,7]
2	$\left[x,\ \frac{1}{4},\ -z\right]$	[2,8]
3	$\left[-x,\ \frac{1}{4},\ -z\right]$	[3,5]
4	$\left[-x,\ \frac{3}{4},\ z\right]$	[4,6]
5	$\left[x+\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[9,15]
6	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[10,16]
7	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[11,13]
8	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[12,14]
9	$\left[x,\ \frac{1}{4},\ z\right]$	[17,23]
10	$\left[x,\ \frac{3}{4},\ -z\right]$	[18,24]
11	$\left[-x,\ \frac{3}{4},\ -z\right]$	[19,21]

continued ...

Table 16

No.	position	mapping
12	$\left[-x,\ \frac{1}{4},\ z\right]$	[20,22]
13	$\left[x+\frac{1}{2},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[25,31]
14	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[26,32]
15	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[27,29]
16	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[28,30]

Table 17: Wyckoff site: 16q, site symmetry: .m'.

No.	position	mapping
1	$[x,\ 0,\ z]$	[1,23]
2	$[x,\ 0,\ -z]$	[2,24]
3	$\left[-x,\ \frac{1}{2},\ -z\right]$	[3,21]
4	$\left[-x,\ \frac{1}{2},\ z\right]$	[4,22]
5	$[-x,\ 0,\ -z]$	[5,19]
6	$[-x,\ 0,\ z]$	[6,20]
7	$\left[x,\ \frac{1}{2},\ z\right]$	[7,17]
8	$\left[x,\ \frac{1}{2},\ -z\right]$	[8,18]
9	$\left[x+\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[9,31]
10	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[10,32]
11	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}-z\right]$	[11,29]
12	$\left[\frac{1}{2}-x,\ 0,\ z+\frac{1}{2}\right]$	[12,30]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[13,27]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[14,28]
15	$\left[x+\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	[15,25]
16	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	[16,26]

Table 18: Wyckoff site: 32r, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[x,\ -y,\ -z]$	[2]
3	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	[3]
4	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[4]
5	$[-x,\ -y,\ -z]$	[5]
6	$[-x,\ y,\ z]$	[6]
7	$\left[x,\ \frac{1}{2}-y,\ z\right]$	[7]
8	$\left[x,\ y+\frac{1}{2},\ -z\right]$	[8]
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[9]
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[10]
11	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[11]
12	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	[12]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[13]

continued ...

Table 18

No.	position	mapping
14	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[14]
15	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[15]
16	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[16]
17	$\left[x,\, y+\frac{1}{2},\, z\right]$	[17]
18	$\left[x,\, \frac{1}{2}-y,\, -z\right]$	[18]
19	$[-x,\, y,\, -z]$	[19]
20	$[-x,\, -y,\, z]$	[20]
21	$\left[-x,\, \frac{1}{2}-y,\, -z\right]$	[21]
22	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[22]
23	$[x,\, -y,\, z]$	[23]
24	$[x,\, y,\, -z]$	[24]
25	$\left[x+\frac{1}{2},\, y,\, z+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27]
28	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}-z\right]$	[29]
30	$\left[\frac{1}{2}-x,\, y,\, z+\frac{1}{2}\right]$	[30]
31	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[31]
32	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[32]